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CUAVA InGaAs-based, Short Wavelength InfraRed (SWIR) instrument for atmospheric reconnaissance: preliminary design



CUAVA InGaAs-based, Short Wavelength Infrared (SWIR) Instrument for Atmospheric Reconnaissance—Preliminary Design

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ABSTRACT

We report the preliminary design of a new small-size remote sensing instrument operating in the Short Wavelength Infrared (SWIR) domain of the spectrum (1.588µm to 1.673µm) to monitor, detect, and measure atmospheric constituents such as Carbon Dioxide (CO₂) and Methane (CH₄) concentrations. We highlight the instrument features, technical specifications (including a relatively high spectral resolution of approximately 0.4 nm), optical design, and components. The instrument's synthetic spectral response is also explored using NASA's Planetary Spectrum Generator (PSG), a Line-by-law radiative transfer code. The instrument is currently under development at the ARC Training Centre for CubeSats, UAVs & Their Applications (CUAVA), and Sydney Astrophotonic Instrumentation Laboratory (SAIL) at the University of Sydney. Once built, it will conduct an atmospheric reconnaissance from an Unmanned Aerial Vehicle (UAV) and will be tested to qualify for future space flights on one of CUAVA's CubeSats.

Keywords: SWIR, NIR, Atmospheric Monitoring, Spectrometer, InGaAs Detector, Remote Sensing.

1. INTRODUCTION

Atmospheric composition has been a continuous target for both long- and short-term studies and analysis due to its critical role in life developing and surviving on Earth^{1,2}. The chemical composition of Earth's atmosphere, in particular, has attracted wide attention from both the atmospheric and space physics community in detecting, measuring, and quantifying atmospheric molecules and suspended particles. Atmospheric molecules such as Carbone Dioxide (CO₂), Methane (CH₄), Water Vapor (H₂O), Carbone Monoxide (CO), and Nitrous Oxide (N₂O) are of particular interest to atmospheric physicists due to their roles in trapping heat in the atmospheric layers³, leading to what is known as global warming⁴⁻⁶.

There have been various instruments designed and developed to enable air- and space-based measurements of atmospheric gases. They can be summarized in two categories: 1) Large instruments with super high spectral resolution and 2) Small instrument with coarse spectral resolutions. Space missions such as Orbiting Carbon Observatory-2 (OCO-2)⁷, Greenhouse Gases Observing Satellite (GOSAT)⁸, SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY)⁹, and Carbon Dioxide Observation Satellite Mission (TanSat)¹⁰ were built with large and custom-made optics and detectors. Their design approach was developed to enable ultra-high spectral resolutions (0.08nm – 0.16nm) from space-based platforms, leading to an expensive budget allocation. On the other hand, small instruments on Nanosatellites such as Argus 1000 micro-spectrometer onboard the second Canadian Advanced Nanospace eXperiment satellite (CanX-2)¹¹ enables miniaturization concepts but comes with coarse spectral resolution (5nm) compared to large space-based instruments. The Greenhouse Gases Satellite (GHGSat), however, is another NanoSat that carries a passive spectrometer with a relatively high spectral resolution (0.1 nm)¹² but is tuned only to detect the atmospheric Methane (CH₄) concentration in the narrow spectral channel 1630 –1675 nm¹³.

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In this paper, we report a small-size, cost-effective instrument that utilizes commercial off-the-shelf components (COTS), i.e., optical elements such as Infrared lenses, and operates in the spectral interval $1.588\mu m - 1.673\mu m$ with a relatively high spectral resolution of approximately 0.4 nm. The instrument will have the capability to detect and measure CO_2 and CH_4 absorption bands simultaneously from an Unmanned Aerial Vehicle (UAV) platform, and will be tested to qualify for a space mission onboard one of CUAVA's NanoSats in the near future.

2. INSTRUMENT

2.1 Optical Design

The instrument is a passive spectrometer operating in the Short Wavelength Infrared (SWIR) part of the spectrum from $1.588 \mu m$ to $1.673 \mu m$. It is intended to conduct the first atmospheric reconnaissance from a UAV platform and be tested to qualify for a future space mission. The instrument specifications are listed in Table 1.

The optical layout of the instrument was designed using OpticStudio[®] ZEMAX software which enables optical simulation. The Instrument optical design mainly consists of five optical elements, slit, collimator, diffraction grating, camera (focusing unit), and detector. Figure 1 shows the instrument's preliminary optical layout produced by Zemax.

Table 1: Instrument parameters

Parameter	Value
Spectral Range	1.588 μm – 1.673 μm (1588 nm – 1673 nm)
Spectral Resolution	0.4 nm
Detector	640 (W) × 512 (L) pixels
Diffraction Grating	600 l/mm (VPH Transmission Grating)
Littrow angle	29°
Slit	25 μm (W) × 3 mm (L)

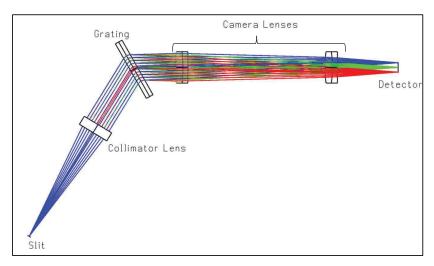


Figure 1: Instrument Optical Layout. Colors represent the wavelengths where Blue is the minimum of $1.588 \mu m$, Green is the central wavelength $1.6305 \mu m$, and Red is the maximum wavelength of $1.673 \mu m$.

2.1.1 Input Slit

Etendue is a significant quantity that defines the amount of light collected by the instrument, and it must be matched for all the optical components in the instrument¹⁴. The following equation describes it as:

$$E = A\Omega \tag{1}$$

where A is the area of the slit surface and Ω is the solid angle at which light is accepted into the instrument.

It is acknowledged that there must be a trade-off between the slit size and the spectral resolution of the instrument to maintain a high signal-to-noise ratio (SNR) with acceptable spectral resolution.

In this instrument, light is collected by a conventional field lens, which must have an F/# of 3.3, and will pass through a 25 μ m slit width that has a length of 3 mm. Figure 2 shows the slit simulation in Zemax. The slit is positioned perpendicular on the transmission grating to enable Littrow condition with an angle of 29°.

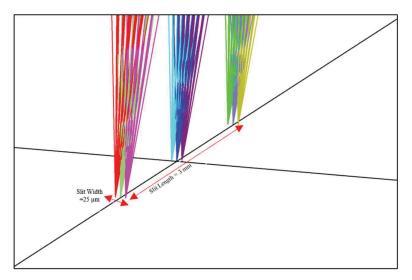


Figure 2: A close-up look at the slit. Slit length is 3 mm, while the width is $25 \mu m$ (0.025 mm). The rectangular slit is simulated to model the light at three different positions in the rectangular. On-axes positions are shown in the middle at three points, one at the centre and two at the edges. Off-axes positions are shown at the two extreme ends of the rectangular slit.

2.1.2 The Collimator, Grating, and Camera

We have experimented with a wide variety of lenses available in Zemax libraries from different manufacturers, e.g., ThorLabs, Edmund Optics, and Newport, and found preliminary suitable optical components for the system. Starting with the collimator, we have selected an achromatic lens coated for the Near Infrared (NIR) and Short Wavelength Infrared (SWIR) bands from Edmund Optics^a. It has a diameter of 30 mm, an effective focal length of 100 mm, and thus an F/# of approximately 3.33. It is shown in Figure 1 as a white rectangle with no further details because the manufacturer only provided a ZEMAX Blackbox of this lens to preserve their intellectual property rights. The collimated light will illuminate a transmission grating (Wasatch Photonics^b) with a 600 line/mm with a diameter of 50.8 mm, which is oriented in a Littrow configuration with an incident angle of 29°. The diffraction grating offers an average efficiency of up to 90% at 1.588 μ m. It, however, drops to approximately 86% at 1.673 μ m, as shown in Figure 3. Diffracted light will then be brought into a focal point at the detector using two achromatic lenses (Edmund Optics) with a diameter of 25 mm. The camera lenses have focal lengths of 200mm and 150mm, respectively, and are separated by a distance of about 108.5 mm resulting in a total effective focal length of 47.9 mm.

a https://www.edmundoptics.com

b https://wasatchphotonics.com

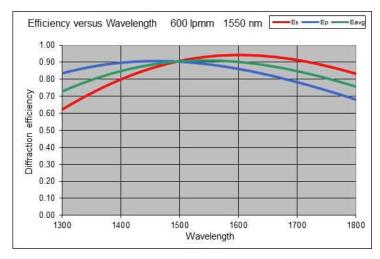


Figure 3: Typical transmission grating efficiency specified by Wasatch Photonics The efficiency of S- and P-type polarized light are shown in red and blue lines, respectively. The average efficiency is shown in the green line. Figure credit: © 2021 Wasatch Photonics.

2.1.3 Detector

An Indium Gallium Arsenide (InGaAs) based detector is a perfect candidate in the SWIR range for its compactness, high Quantum Efficiency (QE)¹⁵ and being the most cost-effective option we have. We aim to employ a high-speed, 640×512 pixels detector with a QE of approximately 70% from the First Light Imaging. It has a length and width of 55 mm and a pixel pitch of 15μ m resulting in an active area that fully accommodates all wavelengths, as shown in Figure 4.

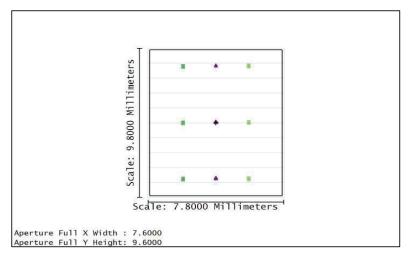


Figure 4: Footprint diagram of the image on the detector. The aperture's full Y height is 9.6mm, representing the 640 pixels. The X width of the aperture (7.6mm) represents the 512 pixels on the detector.

3. PERFORMANCE

3.1 ZEMAX Simulation

The slit is modelled by selecting nine positions (fields), 3 in the middle, 3 in the right, and 3 in the left, as shown in Figure 2. The initial system performance was tested by ray tracing and generating the Spot Diagram of each field position for a range of wavelength, as shown in Figure 6. The columns represent the minimum, central and maximum wavelengths with a spectral step (resolution) of 0.4 nm. The system's minimum wavelength, 1588 nm, is shown in group A and advanced with a spectral step of 0.4 nm twice, giving 1588.4 nm and 1588.8 nm shown in the second and third columns, respectively. The central and maximum wavelengths, 1630.5 nm and 1673 nm are shown in group B and C, respectively, with the same spectral step. The filed positions on the slit are shown in the rows. Group 1 has three positions at the center of the slit. Group 2 and 3 show another 3 points at the right and left edges of the slit, respectively. The spot diagram shows that all rays are confined within the Airy disk with a radius of 12.14 μ m. It is also noteworthy that the spot diagram illustrates a relatively consistent and uniform performance of the system on and off-axis.

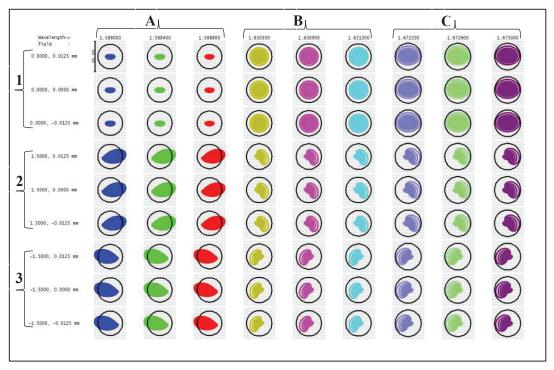
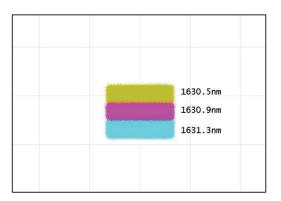


Figure 56: Matrix Spot Diagram of filed positions in slit shown in Figure 2. Columns show the wavelengths 1588 nm, 1630.5 nm, and 1673 nm with a spectral step of 0.4 nm. Rows represent positions selected on the slit center and the two extreme edges. The box size is 30 μm, and the Numerical Aperture (NA) is 0.1.

The system's spectral resolution was tested in ZEMAX by generating the Geometric Image Analysis (GIA) feature, which we use to show the wavelengths separated by the required spectral step can be resolved. Figure 7 shows the central wavelength of 1630.5 nm with two adjacent wavelengths, 1630.9 nm and 1631.3 nm, separated by 0.4 nm spectral step. The normalized radiance profiles of these wavelengths' peaks are shown in Figure 8. The Full-Width-at-Half-Maximum (FWHM) value in figure 8 indicates that the slit image is sampled by at least 2 pixels on the detector.



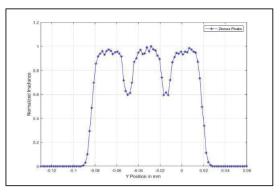


Figure <u>67</u>: Central wavelength 1630.5 nm with two nearby wavelengths, 1630.9 nm, and 1631.3 nm, separated by 0.4 nm.

Figure 78: Normalized Radiance profile of the wavelengths peaks in figure 6

4. SPECTRAL ANALYSIS

4.1 Synthetic Spectral Responsivity

The instrument operates in the SWIR interval $1.588~\mu m - 1.673~\mu m$, which includes some atmospheric molecular absorption bands, mainly CO_2 , CH_4 and H_2O . This spectral domain offers minimal interference by H_2O and relatively high signal-to-noise ratio (SNR) compared to thermal channels. The solar radiance that reflects off the ground and travels back to space carries various information about the atmosphere that can be inferred, i.e., gas concentration, temperature, and pressure. The Planetary Spectrum Generator (PSG)¹⁶ is an online accurate radiative transfer code developed to solve the entire atmosphere's radiative transfer equation. It allows the user to enter all the parameters related to Earth, atmosphere, and instrument. Thus, it has been used to simulate our instrument's spectral range, where data is stored and processed in MATLAB. Figure 9 shows the instrument spectral range that includes absorption bands of CO_2 and CH_4 . Figure 10 shows the gas transmittance in the instrument spectral window. The main atmospheric and spectroscopic parameters used in this Line-by-Line calculation are listed in Table 2.

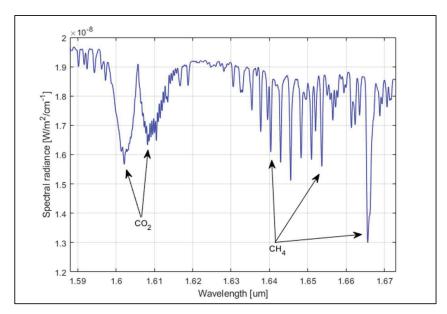


Figure 89: Instrument spectral interval generated by NASA's Planetary Spectrum Generator (PSG). The lines resolution is set to 0.4 nm to simulate the instrument spectral resolution.

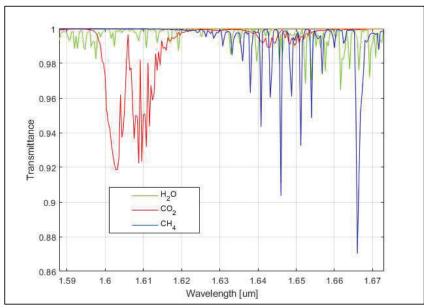


Figure 940: Gases transmission in the atmosphere. CO_2 (red) CH_4 (blue), and H_2O (green), profiles are plotted with standard concentrations in the atmosphere.

Table 2: Calculation parameters used to solve the Radiative Transfer Equation in the synthetic atmosphere.

Parameter	Value
Atmospheric model	Hydrostatic Equilibrium
Spectroscopic Information	HiTRAN 2016.
Albedo	0.31
Surface Temperature	296.54 K
Spectral Range	1.588 μm – 1.673 μm
Spectral Resolution	$0.4 \text{ nm} (1.58 \text{cm}^{-1})$
Observation Geometry	Nadir
Observation angle	31°
Incidence angle:	51.519°

4.2 Retrieval Algorithm

The challenges of retrieving atmospheric constituents from space & aircraft (including UAVs)-based platforms are well known to the Atmospheric and Space physics community. However, much effort has been put into developing retrieval algorithms to meet various mission's needs¹⁷⁻²². These algorithms share a basic fundamental approach that requires forward modelling, but each employs different inversion techniques to infer the atmospheric parameters of interest. The inversion algorithms offer a significant mean to infer specific components from the radiative transfer equation, which is not invertible analytically because of its non-linearity nature.

The adapted retrieval method for the instrument is similar, in concept, to that of OCO-2¹⁸, GOSAT²¹, and SCIAMACHY^{19,20} missions retrievals where the algorithm starts with a forward model that includes instrument parameters to generate a synthetic measurement and ends by employing an inversion method, Optimal Estimation²³, to infer the

atmospheric parameters of interest. Furthermore, the Levenberg–Marquardt inversion algorithm 24 will be evaluated once the flight data is ready for analysis. The forward model can be mathematically represented by the measurement vector, \mathbf{y} as follows:

$$y = F(b, c, x) + \varepsilon$$
 (2)

Equation 2 states that the spectrum (e.g., measurement) \mathbf{y} is a function (\mathbf{F}) of the parameters, \mathbf{b} for the instrument parameters, \mathbf{c} for the known physical parameters, and \mathbf{x} for is the state vector of the target (e.g., the atmospheric gas of interest). The ε term represents the noise or random error in the set of measurements²⁵.

As mentioned previously, to inverse the equation, an iterative retrieval algorithm based on Bayesian optimal estimation²³ will be employed. Bayes's rule finds the probability of a specific event by combining a priori knowledge about the atmospheric state to obtain the posterior state. Bayes's theorem can be implemented, assuming Gaussian statistical distribution, in the retrieval algorithm and the maximum posterior probability state $\hat{\mathbf{x}}$ and its covariance matrix $\hat{\mathbf{S}}$ are:

$$\chi^{2} = (\mathbf{y} - \mathbf{F}(\mathbf{x}))^{T} \mathbf{S}_{\varepsilon}^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x})) + (\mathbf{x} - \mathbf{x}_{a})^{T} \mathbf{S}_{a}^{-1} (\mathbf{x} - \mathbf{x}_{a})$$
(3)

$$\mathbf{S} = (\mathbf{K}^T \mathbf{S}_{\varepsilon} \, \mathbf{K} + \, \mathbf{S}_a^{-1})^{-1} \tag{4}$$

where the **x** and **y** are the state vector and measured spectrum, respectively, illustrated in Eq. (2), \mathbf{S}_{ε} is the measured error covariance, \mathbf{x}_a and \mathbf{S}_a are the priori state vector and priori covariance matrix, T is the transpose operator, **K** is the weighting function¹⁸ and $\mathbf{F}(\mathbf{x})$ is the forward model expressed in Eq. (2).

5. CONCLUSION

We have reported a new small size, passive remote sensing instrument operating in the Short Wavelength Infrared (SWIR) with a relatively high spectral resolution of approximately 0.4 nm to monitor, detect and measure CO_2 and CH_4 concentration in the lower atmosphere. We have shown the instrument preliminary optical design and performance in ZEMAX and simulated its spectral responsivity utilizing the Planetary Spectrum Generator (PSG), a line-by-line radiative transfer code developed by NASA. The filed lens, which determines the field of view (FOV), will be selected, and the whole system will be tested again in ZEMAX. Initially, the instrument will conduct its first reconnaissance from a UAV platform and collect data over various targets on the ground. It will, then, be tested to qualify for a space mission onboard one of CUAVA's future CubeSats.

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